NON-LINEAR MODELLING OF BIOLOGICAL ACTIVITY OF CHEMICAL COMPOUNDS

ABSTRACT OF THE DISCLOSURE

Models predict activity of chemical compounds by employing "transformed" descriptor values. The descriptors are transformed via transformation functions that convert the raw descriptor values to new values better representing the contribution of the descriptors to the activity in question. Typically, these transformation functions are non-linear parametric functions such as Gaussian functions or sigmoid functions. Typically, the model will employ at least two different descriptors, each transformed by its own non-linear parametric function.